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# MULTISCALE MODELING FOR THE DESIGN OF AUTONOMIC HEALING STRUCTURAL COMPOSITE MATERIALS (MEANS)

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We developed a suite of molecular-scale simulation tools, which includes all-atom MD simulations and coarse-graining procedures to interface with CVFE calculations at the continuum level. Polymerization reaction mechanisms and rates are identified in all-atom simulations. A first coarse-graining procedure consists of eliminating atoms that are unimportant for the mechanical properties of the structure. In a second coarse-graining procedure representation of monomers is simplified to spherically symmetric particles. This allows one to generate large-scale realistic polymer networks and predict the mechanical properties of polymer structures with specific chemistries. This computational approach was validated by studying polymerization of DCPD under strain. Conclusions are: (i) the numerical acceleration of the reaction and transport processes does not alter the network structure; (ii) the mechanical properties are independent of the catalyst concentration and reaction rates; (iii) reproducing the underlying reaction mechanisms correctly at the molecular level is essential to generating realistic network structures and predicting materials properties.

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## Executive Summary

This MEANS initiative research project consists of a collaborative effort between students, postdocs, and faculty at the University of Illinois and at the University of Michigan. The work involves the integration of length and time scale spanning computational methods of investigation into a suite of design tools for materials optimization. Concurrent experimental measurements serve to motivate and validate the simulation approaches. Specifically, the challenges posed by the design of autonomously healing polymer matrix composites[1] were chosen as the test case for the development of this computational framework, which includes reactive molecular dynamics (MD) simulations, coarse-grained particle-based simulations, and cohesive-volume finite element (CVFE) calculations. The integration of the different methodologies is achieved through data exchange and output overlap matching.

We developed a suite of molecular-scale simulation tools, which includes all-atom MD simulations and two coarse-graining procedures, and which interfaces with CVFE calculations at the continuum level. The all-atom simulations allow us to identify the reaction mechanisms and the reaction rates that underlie the formation of the cross-linked polymer network. The first coarse-graining procedure, which consists of eliminating atoms that are unimportant for the mechanical properties of the structure, allows us to characterize the topology of the network that develops and calibrate elastic constants and bond strengths. The second coarse-graining procedure, which consists simplifying the representation of monomers to that of a spherically symmetric particle, allows us to generate large-scale realistic polymer networks based on construction rules derived from the finer-grained levels of simulation, and predict the mechanical properties of structures derived from monomers with specific chemistries.

We validated our computational approach by studying polymerization of DCPD under strain and conclude that: (i) the numerical acceleration of the reaction and transport processes does not alter the network structure; (ii) the mechanical properties are independent of the catalyst concentration and reaction rates; (iii) reproducing the underlying reaction mechanisms correctly at the molecular level is indeed essential to generating realistic network structures and predicting materials properties.

## 1. Introduction

In self-healing materials an autonomous repair process is triggered by a fracture event. This mechanism is realized by embedding repair agents, encapsulated in thin-walled microscopic spheres, and chemical initiators into a polymer composite structural matrix. The matrix is the structural (load-bearing) material in this design. The embedded microcapsules, even without releasing the repair agent, already enhance the material's toughness. When a crack approaches the embedded microcapsule, causing it to rupture, the repair agent inside the microcapsule is released and wicked into the crack plane through capillary action. Once the repair agent reaches the crack plane an embedded catalyst initiates a polymerization reaction and solidifies the repair agent in place. Under cyclic loading conditions, this mechanism can reestablish cohesion in regions through which the crack has already passed. Fabrication, testing, and evaluation of such materials require extensive experimentation cycles. Numerical simulation is instrumental to accelerating the development of such materials systems, first by allowing one to gain a better understanding of the fundamental processes that control the behavior of the material during operating conditions, and ultimately as predictive design tool.

## 2. Objectives

The purpose of this project was to create a multi-scale computational framework for the design of complex materials systems by integrating molecular dynamics simulations based on a reactive force field, cohesive/volumetric finite element calculations, and a particle-based coarse-grained model to bridge the gap between atomistic and continuum modeling techniques. The particular challenge in developing this computational framework arises from the necessity to simulate the materials response to mechanical loading on a macroscopic timescale while the structural developments associated with the healing processes require resolution of mechanisms at atomic time and length scales.

While the focus for this project was on self-healing materials systems, the fundamental research pursued in this project yielded tools of analysis and experimental databases that impact materials applications beyond self-healing. The multi-scale simulations that we developed have utility in the design of composites and multiphase materials for enhanced fatigue life and increased fracture resistance. The molecular dynamics simulations of *in situ* reaction and transport phenomena, while examining the stiffness and strength of the resulting structures, have broad applicability in the field of polymer processing and process modeling, especially in the development of structural materials.

## 3. Approach and Methodology

The design of self-healing materials systems requires very detailed and careful optimization of processes, including the choice of materials and repair agents based on their physical, chemical, and kinetic properties, as well as geometric and structural considerations at various levels. On the one hand, the properties of a material are very fundamentally rooted in the structure and dynamics of its atomic-scale constituents. On the other hand, the actual materials performance depends on a complex scale-spanning hierarchy of such elementary mechanisms. Incorporating atomically resolved processes

in a modeling framework therefore provides for greater realism and accuracy in predicting materials behavior. At the same time one needs to keep track of how progressions of elementary processes compound into macroscopic observables. Computationally, this requires one not only to encompass the pertinent length scales and spatial resolution, but importantly, the time scales corresponding to the reaction between molecular building blocks and to the fatigue crack propagation must be reconciled.

To create a suitable multi-scale design tool we combined explicit-atom molecular dynamics (MD) simulations with continuum-scale cohesive/volumetric finite element (CVFE) calculations. Furthermore, to overcome the time-scale disparity between these two methods, we have developed a coarse-grained particle-based (CGP) simulation procedure that allows one to simulate atomic-scale processes in an accelerated fashion by abstracting structural detail at the building block level. CVFE is used to model fatigue crack propagation at the macro-scale. This part of the project was carried out in the group of Prof. Geubelle at the University of Illinois, while our group at the University of Michigan worked on the atomistic and intermediate-scale simulations. This report focuses on the molecular-scale simulation aspects of the computational framework. MD simulations are used to simulate the structural aggregation upon curing of the healing agent, determine reaction rates, and establish the relationship between mechanical properties and molecular structures at various stages of the curing process. Molecular-scale simulations furnish the loading rate dependent constitutive behavior needed as input for the cohesive volume elements continuum calculations. Conversely, CVFE establishes the local conditions under which the molecular state of the material is to be evaluated.

While it is generally possible to simulate molecular structures large enough to yield local properties that are representative of the macroscopic materials behavior, a serious limitation in connecting atomistic and continuum scales arises when structural changes result from macroscopic mechanical loading that is many orders of magnitude slower than atomic motions. Particularly, the macroscopic failure process, curing rate and deformation rate in self-healing composites compete on time scales not attainable by MD simulations. Moreover, the deformation and failure may induce structural defects whose spatial extents exceed those of MD simulation boxes. Therefore, we inserted an intermediate-scale lattice-based modeling approach to bridge between atomistic and continuum scales.

The development of our simulation framework was closely coupled with the experimental work of Profs. White and Sottos at the University of Illinois. This collaboration allowed us to identify the design issues that need to be addressed by our numerical tools and provided us with experimental data to properly validate our modeling efforts.

## 4. Accomplishments

Our molecular-scale simulation approach encompasses three levels: (i) a fully atomistic level, where all atoms contained in the system are explicitly represented. At this level we identify reaction mechanisms, determine reaction rates, and gain structural information; (ii) a first coarse-graining level, in which larger polymeric networks are generated and the relationship between structure and mechanical properties are determined; and (iii) a

second coarse-graining level, where reaction rates and deformation rates are reconciled and the overall mechanical response of the healing agent under application conditions is determined. The development of individual simulation techniques, i.e., the reactive MD simulations and the CGP model, has been completed. The methods have been applied to study the autonomous repair behavior of self-healing polymer composites under strain.

### 4.1 Accomplishment in Atomic-Scale Simulations

Polymerization and cross-linking reactions have been successfully reproduced in atomic scale simulations for systems of several hundred monomers. These simulations revealed the reaction mechanism and polymerization rates. The dicyclopentadiene (DCPD) molecule posses two reactive sites, i.e., the C=C double bonds on the buckled hexagonal ring and the pendant cyclopentenyl ring (see fig. 1). Both rings are subject to ring-opening methathesis polymerization (ROMP), which is invoked by a catalyst, e.g., the transition metal complex Ru(arene)$Cl_2(PCy_3)$.[2,3] The MD simulations using our reactive force field,[4,5] reproduce both ring opening mechanisms. Our simulations show that because the hexagonal ring is subject to significant strain, it is considerably more reactive and hence, the polymerization initially leads to linear chains. Cross-linking sets in at a slower rate, as controlled by the opening of the cyclopentenyl rings. This confirms the prevalent views concerning this mechanism as described in the literature.[2] Importantly, through simulation of the detailed bond formation processes we are able to generate a realistic model of a polymeric DCPD network, and establish its structure property relationships. In particular, using this level of simulation we can determine the reaction rate coefficient that describes the polymerization reaction. This only requires a few hundred monomers, for as long as all steric arrangements that can occur during the polymerization are represented in the simulations. This is readily achieved by studying a series of structures with different initial configurations.

Explicitly accounting for hydrogen in the simulations is costly in terms of computing times, not only because of the mere number of atoms to keep track of, but because of the small mass of hydrogen, the integration time step needs to be drastically reduced for the simulation scheme to produce accurate trajectories. Structurally, hydrogen plays a secondary role, e.g., it has negligible load bearing function, and it is therefore common practice to account for hydrogen atoms implicitly by reconfiguring CH and $CH_2$ groups into unified particles, as shown in fig. 1. These new units are characterized by sizes and

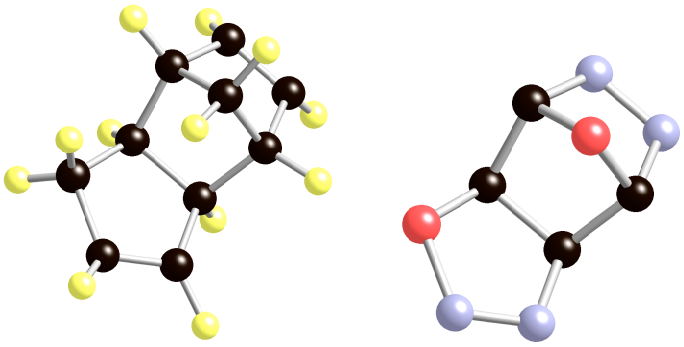



**Fig. 1** Simulated DCPD molecule, (a) with all atoms represented explicitly, and (b) with hydrogen atoms treated implicitly. This reduced form of the molecule contains three types of hydrocarbon croups $sp^3$ $CH_2$ (red), $sp^3$ CH (black), and $sp^2$ CH (blue). Reactive sites are the double bonds between $sp^2$ groups.

chemical interactions representative of the steric functionality of the groups that they replace. We have developed a model of DCPD molecules following this scheme and ascertained that the polymeric networks that form have the same geometry as those resulting from all-atom simulations. Fig. 2 shows an example of a simulation result using this simplified model of DCPD monomers.

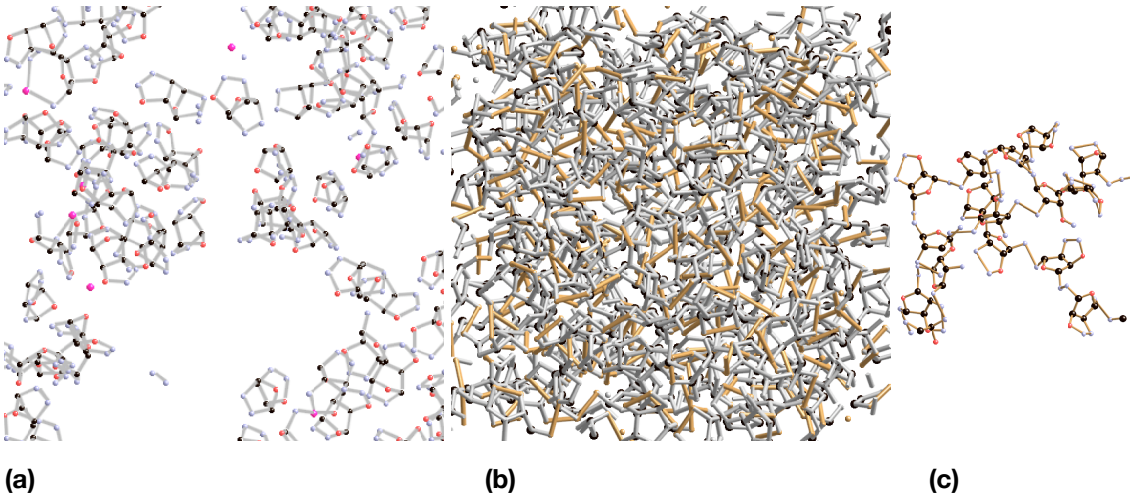



**Fig. 2** Simulated polymerization of DCPD based on the unified building blocck approach: (a) initial configuration of monomers and catalysts; (b) network formed after 2 ns at 500 K (c) fragment of a polymerized DCPD network, with unreacted monomers omitted for clarity.

This simplified representation of the DCPD molecule results in an increase of computational speed by nearly an order of magnitude. Accordingly, it allows for an increase in the size of simulated structures, yielding improved statistics in the description of the resulting network topologies. Based on this first coarse-graining step, we can generate polymeric networks ultimately containing several ten thousand monomers and study their structure and properties under conditions that represent all possible states the healing agent can achieve between initiation and completion of the polymerization, assuming various degrees of mechanical deformation. The important measure that results from this level of simulation is the relationship between structure and mechanical properties of the polymer network. In particular, we can determine elastic moduli and tensile strengths of networked structures at various densities. Variable density, in this case, corresponds to situations where completion of the polymerization reaction was achieved at different degrees of strain in the system.

### 4.2 Progress in Coarse-Grained Simulations

The simulation times that can be achieved at the aforementioned level, however, are far shorter than would be required to cover the experimental deformation rates. To realistically accommodate simultaneous deformation and polymerization as the factors contributing to the structural evolution of DCPD networks, a second level of coarse graining has been introduced, i.e., the CGP procedure. At this level, each DCPD monomer is represented by a single particle that can move about, and upon collision with other units it can undergo a polymerization reaction depending on whether the conditions

for this process to occur are fulfilled. These conditions are known from atomistic simulations, and accordingly we developed statistical rules for structural evolution that are implemented via a Monte Carlo numerical procedure. These rules, obviously, are designed to maintain realism in the simulated polymerization process. E.g., at least one of the particles must carry the Ru catalytic complex. Upon reaction, the Ru complex residing with the most recently polymerized unit is now transferred to the next monomer that attaches to the chain. This provides for an interesting aggregation scheme, described by the propagation of the catalyst along the growth path of the polymer. Furthermore, at most four other units can attach to any given monomer, and we distinguish between polymerization and cross-linking reactions based on their variable rates.

Unreacted monomers move according to a regular MD algorithm, based on interactions that are described by a shallow Lennard-Jones potential. This shallowness allows for relatively large integration time steps. In fact, in CGP simulations we do not attempt to reproduce the vibrational motion of non-bonded particles, but calibrate the time scale by matching the mean squared displacement of particles in the diffusive regime with that of the center of mass of monomers in explicit-atom MD simulations of DCPD. Upon polymerization, a different potential becomes effective between bonded monomers. This potential has a much deeper well, commensurate of the bonding energy. The curvature at this well's bottom governs the elastic properties of polymer network.

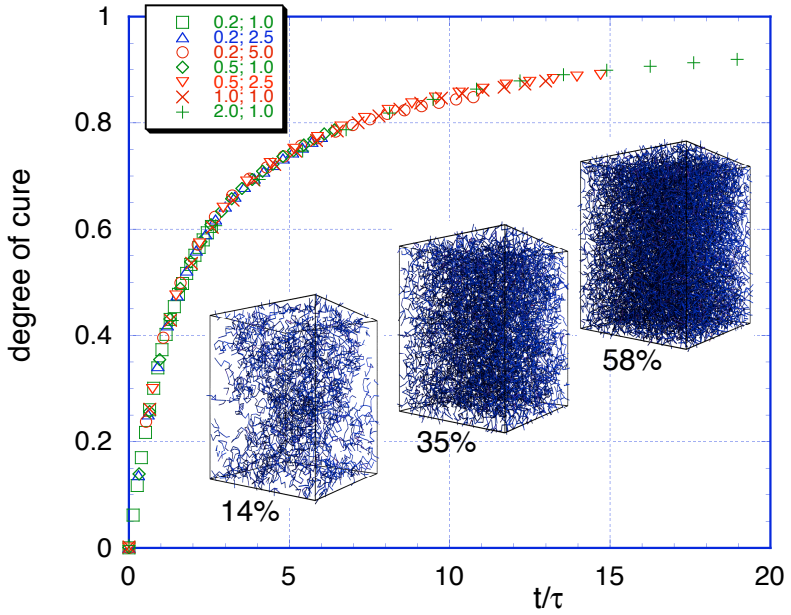



Fig. 3 Degree of cure as a function of scaled time for catalyst concentrations ranging from $0.2 \leq c_{Cat.} \leq 2.0$ and reaction to diffusion rate ratios ranging from $1 \leq k/D \leq 5$. Different symbols represent data obtained for different conditions. Numbers in the legend represent catalyst concentration and reaction to diffusion rate ratio.

The CGP method has been most effective for studying the structural development of the polymerizing healing agent, as well as the ensuing evolution of mechanical properties, because of the large system sizes and long time spans that can be accommodated in at this level. We found that for optimal utilization of the healing agent, it is imperative to embed the catalyst in such a way that it dissolves rapidly and be evenly distributed throughout the DCPD fluid before polymerization reaches significant degrees.

Otherwise, the catalyst may become trapped and rendered ineffective. Alternatively, it may be necessary to slow the polymerization rate, e.g., by increasing the fraction of endo-modification of DCPD in the healing agent.

We have studied these structure-property relationships by systematically varying the ratio of reaction to diffusion rates (cure conditions), as well as the catalyst concentration (design parameter). In general, the degree of cure advances more rapidly the higher the reaction rate is relative to diffusion coefficient and the higher the catalyst concentration. Fig. 3 shows the temporal evolution of the degree of cure for various catalyst concentrations and reaction to diffusion rate ratios. As is shown, by scaling time such that $t' = t/\tau = kt$, all data can be made to collapse onto a master curve that obeys the rate equation $\frac{d\alpha}{dt} = k\alpha^n (1-\alpha)^m$, with $n$ = 0.05 and $m$ = 2.0. Accordingly, this rate equation, which is known as the Prout-Tompkins model, universally describes the polymerization behavior of DCPD, regardless of the magnitude of the overall reaction rates.

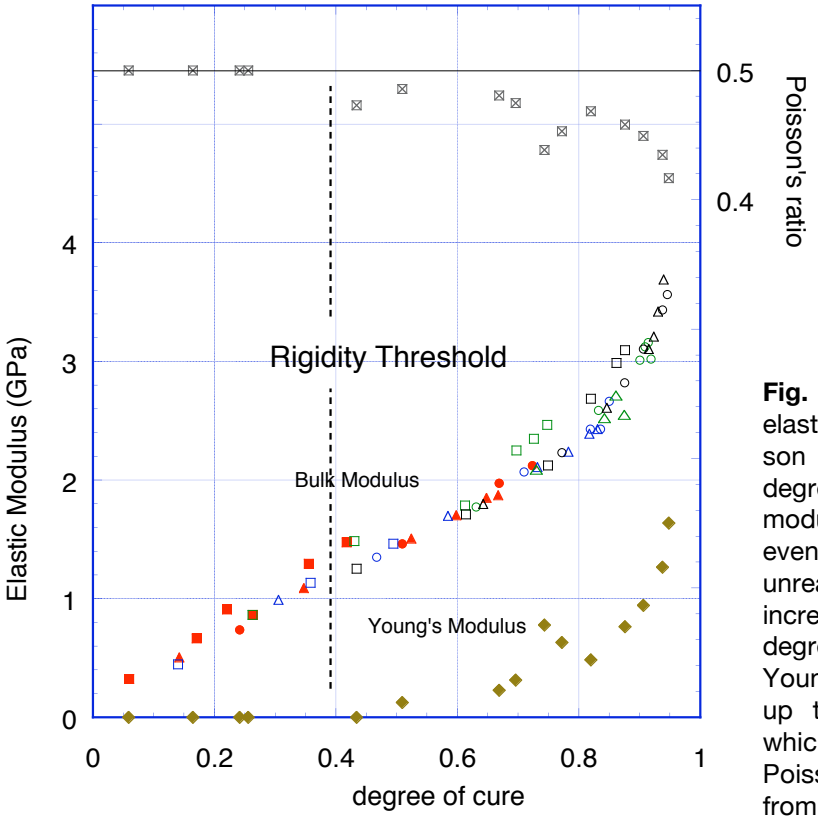
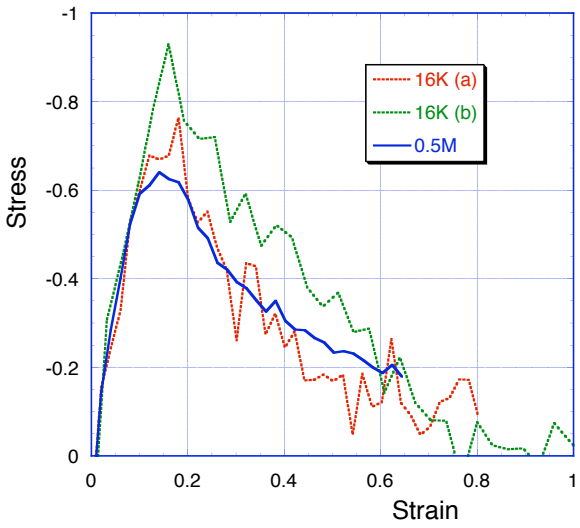



**Fig. 4** Bulk and Young's elastic moduli, and the Poisson ratio as a function of the degree of cure. The bulk modulus has a finite value even when DCPD is fully unreacted (i.e., a liquid), and it increases steadily with the degree of polymerization. The Young's modulus is vanishing up to the rigidity threshold, which is also where the Poisson ratio starts to deviate from that of a liquid.

Furthermore, based on two-point spatial correlations, all of these structures appear to be similar. However, since the structures are amorphous, this is not necessarily a guarantee the structures are actually the same. It is therefore more informative to deduce the relationship between these structures from their mechanical properties. In fig. 4 we compare the bulk modulus of a series of polymerized DCPD structures as a function of the degree of cure. Again, the reaction to diffusion rate ratio has been varied between 1.0

and 5.0, and the catalyst concentration between 0.2 and 2.0 mol%. The degree of cure achieved for different sets of parameters overlap with each other, depending on the time allowed for reaction in each case. This way, the mechanical properties for a given degree of cure, but for different reaction conditions can be directly compared. Interestingly, the modulus vs. degree of cure data for all cure conditions follow the same master curve: initially the modulus depends almost linearly on the degree of cure and then accelerates once more than half the possible network bonds have formed.

This is an important finding not only because it provides one of the data connections to the continuum mechanical calculations that are part of this computational framework,[6] but also because it provides a fundamental understanding of the structural evolution as a function of the degree of cure and the ensuing mechanical properties. Essentially, the elastic properties of polymerized DCPD are independent of the rate of the cure reaction. As an added benefit, this finding justifies acceleration of the simulated polymerization and cross-linking reactions without detriment to the physical significance of the mechanical behaviors of the structures so obtained.



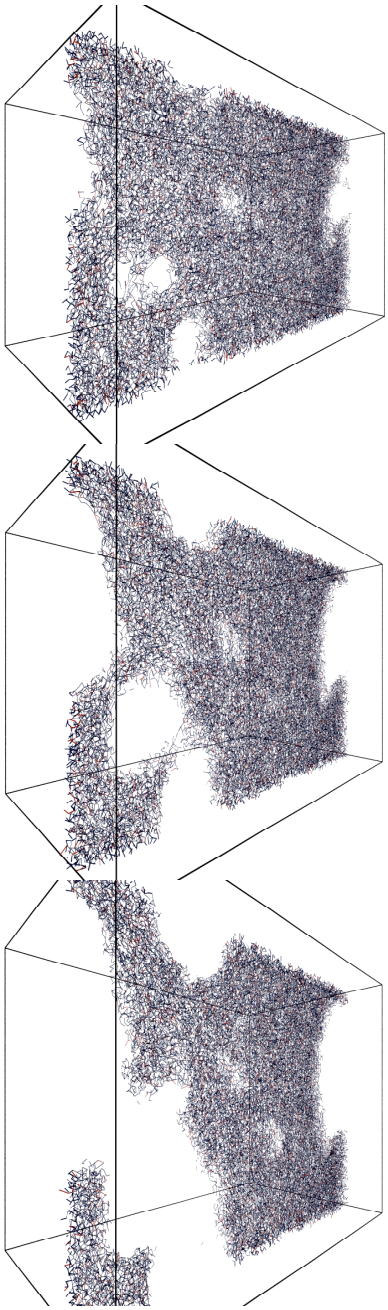



**Fig. 5** Left: Cohesive law of DCPD systems subject to a constant strain rate of $10^5$ $s^{-1}$. One configuration contains 16000 monomers and the other one half a million. Depending on the starting configuration, significantly different yield stresses are achieved in the smaller system. Right: Three frames showing a cross-linked DCPD network at consecutive stages during fracture (only a thin slice of the structure is shown).

One of the key pieces of information of the molecular-scale simulations is the cohesive law (or traction-displacement relationship) needed as input to the CVFE calculations. The coarse-graining scheme has allowed us to simulate much larger systems and accommodate realistic strain rates. In fig. 5 we compare typical cohesive laws obtained for a 16000-monomer system and a half a million-monomer system. The curve for the larger system exhibits fewer fluctuations. Also, different starting configurations, albeit with the same degree of cure, show different yield strengths, which attests to the poor statistics obtained within the smaller system.

Finally, the reason for developing this molecular simulation suite was to predict materials properties and behaviors based on reproducing all pertinent details of the processes that lead to the healing agent's final structure under various thermo-mechanical conditions. One essential question has been how detailed an adequate model needed to be, i.e., whether it matters to simulate a particular reaction process at the molecular scale and obtain a realistic description of the ensuing structure, or whether it would be sufficient to base models on more global descriptors, e.g., the degree of cure, without resolving molecular details of the structure.

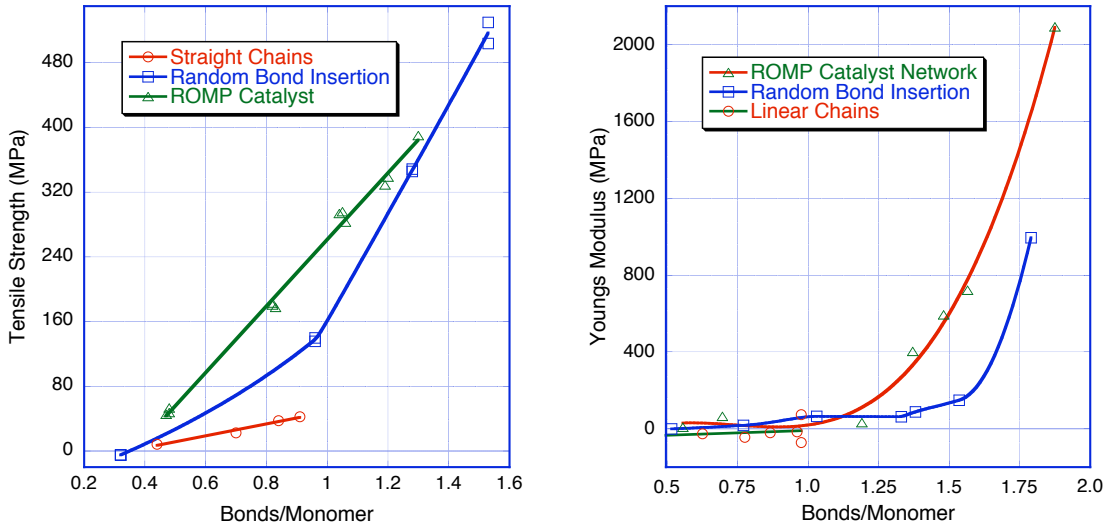



**Fig. 6** Tensile strength and Young's modulus of DCPD networks generated by three different processes, as a function of the degree of cure.

To answer this question, we simulated the formation of a DCPD network in three different ways and calculated the mechanical properties of the resulting structures. One way is accurately reproduce the ROMP reaction mechanism in our simulations, as described above. Note that ROMP mechanism has a peculiar way of propagating the catalyst from one DCPD unit to the next one that attaches to the network. Hence, the configuration of bonds in the network essentially describes the trajectory of the catalyst through space. In our simulations we observed that cross-linking reactions occur about five times slower than linear chain polymerization. Once the majority of linear bonds have formed, cross-linking reactions catch up, so that in systems with high degree of cure, the number of cross-links lies between 50% and 70% of the number of linear bonds.

This represents the network topology we expect in real DCPD. For comparison, we created a second network topology, simply by suppressing cross-link reactions. This leads to the formation of linear chains only. The third procedure we employed was to insert bonds randomly, i.e., whenever two monomers came within bonding distance of each other the algorithm inserted a bond with certain probability and as long as the maximum number of bonds per monomer did not exceed four. We then calculated the yield strengths and the elastic moduli of these structures as a function of the degree of cure (expressed as number bonds per monomer). The results are shown in fig. 6.

The network created through the ROMP process has the highest tensile strength and elastic modulus. Linear chains only react up to one bond per monomer; they have low strength and flow under uni-axial tension. Networks created by random bond insertion overall lower strength than ROMP derived ones, but eventually catch up when the degree of reaction approaches saturation. However, the random bond networks consistently have a lower Young's modulus compared the ROMP structures. While these findings reveal very interesting materials design issues, they also demonstrate the need for the molecular simulations in order to accurately predict materials behavior. Without accurately reproducing the processes that lead to the formation of materials structures, the resulting structural models will be faulty and we will not predict the correct materials properties.

## 5. Conclusions

We have developed a suite of molecular-scale simulation tools, which includes all-atom MD simulations and two coarse-graining procedures, and which interfaces with CVFE calculations at the continuum level. The all-atom simulations allow us to identify the reaction mechanisms and the reaction rates that underlie the formation of the cross-linked polymer network. The first coarse-graining procedure, which consists of eliminating atoms that are unimportant for the mechanical properties of the structure, allows us to characterize the topology of the network that develops and calibrate elastic constants and bond strengths. The second coarse-graining procedure, which consists simplifying the representation of monomers to that of a spherically symmetric particle, allows us to generate large-scale realistic polymer networks based on construction rules derived from the finer-grained levels of simulation, and predict the mechanical properties of structures derived from monomers with specific chemistries. We validated our computational approach by studying polymerization of DCPD under strain and conclude that: (i) the numerical acceleration of the reaction and transport processes does not alter the network structure; (ii) the mechanical properties are independent of the catalyst concentration and reaction rates; (iii) reproducing the underlying reaction mechanisms correctly at the molecular level is indeed essential to generating realistic network structures and predicting materials properties.

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## 6. Interactions/Transitions:

a. Participation

AFOSR Contractor's Meeting on Mechanics of Materials and Devices & Structural Mechanics, September 25-27, 2002, Rosslyn, VA; Presentation title: "Multi-scale Modeling for the Design of Autonomic Healing Structural Composite Materials."

AFOSR MEANS Workshop, Boulder, CO, August 6–8, 2003; Presentation title: "Multi-scale simulation of chemically reactive materials systems."

AFOSR Contractor's Meeting, September 8-11, 2003, Santa Fe, NM; Presentation title: "Multiscale Modeling for the Design of Autonomic Healing Structural Composite Materials."

AFOSR-MEANS Bidder's Meeting, May 3, 2004, Arlington, VA

AFOSR Program Review on "Mechanics of Materials and Devices." August 18-20 2004, Wintergreen Resort, VA. Presentation title: "Multiscale Modeling for the Design of Autonomic Healing Structural Composite Materials."

4th Airforce Workshop on Multi-Functional Aerospace Materials and Structures: Autonomic Response to Damage and Heat, August 8-9, 2005, Urbana, IL; Presentation title: "Systems Design Based on Molecular Simulations."

AFOSR Contractor's Meeting, Aug. 28-Sept. 2, 2005, Santa Fe, NM; Presentation title: "Multiscale Modeling for the Design of Autonomic Healing Structural Composite Materials."

b. Transitions

This work constitutes a part of a multi-investigator effort to bridge length and time scales in materials simulation. Our group works on the atomic-scale and mesoscale simulation of the curing process in the healing agent of a self-healing polymer composite material under various loading conditions. The outcomes of our simulations are the constitutive law for the polymer and healing rate coefficients, which serve as input to the continuum mechanical calculations carried out by Prof. P. Geubelle and his group at the University of Illinois.

New collaborations with Dr. Ajit Roy from the Air Force Research Laboratory at Wright Patterson Air Force Base and Prof. Somnath Gosh from Ohio State University have been developed.